NOVEMBER ISSUE 1999

DATELINE LOS ALAMOS

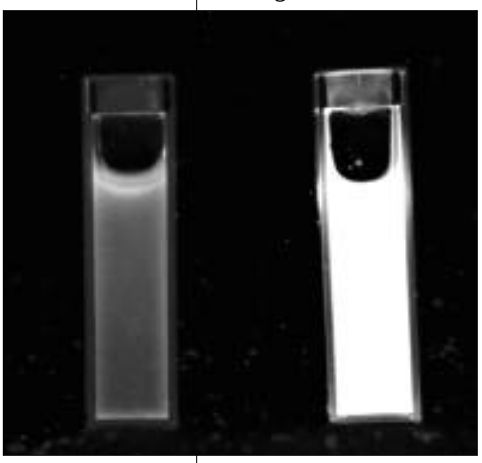
U.S. DEPARTMENT OF ENERGY
UNIVERSITY OF CALIFORNIA

LUMINESCENT SENSORS

NEXT-GENERATION SENSORS MAY DETECT CHEMICAL AND BIOLOGICAL AGENTS, VIRUSES, BACTERIA

It started out as a three-year project to study electron transfer in conducting polymers for possible applications in photovoltaics and nonlinear optics. Then it became something much more significant.

Los Alamos researchers Liaohai Chen, Duncan McBranch, Hsing-Lin Wang and David Whitten, along with researchers from the University of California, Los Angeles, discovered they can create polymeric luminescent sensors capable of detecting biological and chemical agents. These sensors also may be able to detect different types of viruses such as influenza and HIV, as well as bacteria and proteins.



The strong fluorescence of the biosensing polymer-QTL solution appears in the vial on the right when the receptor protein is added.

A paper detailing this finding was published in October in the *Proceedings of the National Academy of Sciences*.

Recently, McBranch and his colleagues have successfully built a portable device to demonstrate their luminescent biosensors. Using a

laptop computer, hand-sized spectrometer, fiber-optic cabling and a cuvette (sample holder), they demonstrated how a polymer's luminescence can be "turned on" by adding a sample protein (avidin, derived from egg whites).

This significant achievement could pave the way for development of a lightweight, portable, real-time diagnostic tool that can be used in private homes, clinics and in the field.

The researchers' work is based on their discovery that certain polymers have an amplified sensitivity to charge transfer — the process by which a conducting polymer's electrons can hop to an electron-accepting molecule such as carbon-60 (C_{60}) or methyl viologen — when excited by light.

However, the polymer loses its luminescence once it transfers its electrons to that acceptor molecule; that is, the polymer's luminescence is quenched. To harness this effect for sensing, the researchers linked the molecular quencher with a specific ligand to create a new molecule known as a quencher-tether-ligand, or QTL. This QTL is the crucial component for selectively detecting and identifying chemical and biological agents. A ligand is any atom or molecule that's attached to a central atom in a molecular compound.

The process is analogous to a lock and key. The ligand part of QTL is the "key," which fits into a receptor site, or "lock," on the biological species to be detected. This recognition event literally pulls away the QTL from the polymer, thereby restoring the polymer's luminescence.

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All pathogens, proteins, viruses and bacteria contain receptor sites, which allow them to latch onto specific ligands (thereby providing a route for infecting cells). By matching the right ligand to receptor, researchers positively can identify that protein, virus or bacterium.

To demonstrate the portable device, McBranch and his colleagues placed a water-soluble, quenched polymer inside the cuvette attached to one end of a fiber-optic cable. The other end is connected to the spectrometer which, in turn, is connected via another cable to the laptop computer.

Los Alamos researcher Liaohai Chen holds a vial of the fluorescent biosensing polymer.

The water-soluble polymer is essential, because the polymer contains negative charges, which attract the positively charged QTL. In the demonstration, the QTL contained the ligand biotin. Biotin/avidin is a well-known ligand/receptor combination that is often used for biochemical binding studies.

Next, the researchers added to the cuvette a solution containing avidin. As expected, the receptors within the protein latched onto the QTL and pulled it away from the polymer. The spectrometer picked up the restored luminescence signal from polymer and displayed it on the computer screen, confirming the presence of those proteins. The analysis and identification process took about a second to complete.

McBranch says if a researcher or physician is not sure what bacteria or viruses are present, he or she simply places a sample into an array of cuvettes containing different, receptor-specific QTLs. The spectrometer would analyze each cuvette simultaneously and again require only seconds to identify the particular species of interest.

The research received initial funding from the Laboratory-Directed Research and Development Program. For more information on LDRD research at Los Alamos, see the August 1999 issue of *Dateline: Los Alamos*. The next step for the researchers is developing a library of different QTLs. They currently are looking for additional funding to create such a library and to further downscale their biosensor device.

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DATELINE: LOS ALAMOS

SAFEGUARDING RUSSIAN NUCLEAR MATERIALS

DOE TEAM HELPS RUSSIA EVALUATE Y2K RISK AT NUCLEAR SITES

When the calendar flips to the year 2000, computer specialists worldwide will be focused on the health of their machines and networks — the Y2K challenge has their complete attention. But arguably none will be more focused than Benny Martinez. He's a Los Alamos computer scientist watching 10 Russian nuclear sites and their nuclear materials protection, control and accounting equipment.

Benny Martinez (third from left) is helping Russian nuclear sites ready themselves for Y2K. This photo was taken on one of Martinez' earlier trips to Moscow in front of an historical church in the Institute of Technical Engineering and Physics compound.

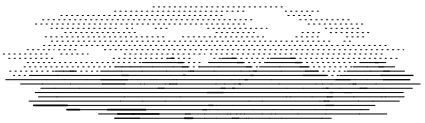
Martinez knows that if a Russian system goes down, its computer-guided cameras, gates or inventory systems become inoperative, nuclear materials could be at risk — and he's not going to let that happen.

The Department of Energy has been putting safeguards upgrades into Russian nuclear facilities for nearly five years as part of an agreement that helps keep nuclear materials out of the hands of rogue nations or terrorists. And in this high-tech world, that means scores of computers and bushels of software are in place. They guide alarm systems and cameras, control checkpoint equipment and total up every precious ounce of uranium and plutonium in the Russian vaults, day by day.

Basically, the new gear brings Russian nuclear materials under the kinds of protection that the United States knows, uses and has faith in.

But the computer world has been rocked by the realization that when internal computer calendars, especially older ones, change from 1999 to 2000, the machines may believe that it's the year 1900. And a plethora of unintended shutdowns, data errors and general confusion may result.

With that in mind, the DOE set up a team to analyze, test and correct equipment at such nuclear sites as Dimitivograd State Scientific Center, Research Institute of Atomic Reactors, the Luch State Research Institute and the Beloyarsk Nuclear Power Plant.



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Martinez, of Los Alamos' Nonproliferation and International Security Division, is the only national laboratory scientist on that team, and as its leader, he has a daunting task, but a certain level of optimism, he says. Since much of the U.S.-provided equipment is fairly new, in theory it is unlikely to suffer a date-related breakdown. But where Russian equipment or parts have been substituted, or where older computers are in place, the need for vigilance is far greater.

Working with the Russian institutions is more than a matter of merely sending Martinez and his team of industrial partners on a whirlwind tour of potential crash sites with a suitcase full of fix-it tools. Martinez notes that much of the effort is being placed in heightening Russian awareness and training the staff of each institute. Throughout August, Los Alamos hosted groups of Russian scientists and technicians for training in the very issues Martinez is worrying about.

The Y2K team returned to Russia in mid-September to conduct on-site evaluations of three facilities in and around Moscow and two facilities in St. Petersburg. During the evaluations, the team collected manufacturers' model numbers and versions of equipment and tested as many systems as possible.

Testing all of the systems at some of the Russian facilities wasn't possible because of the heightened security restricting access to critical areas that has been implemented due to recent bombings in Russia. Of the systems tested, a few older, noncritical personal computers at one facility were not Y2K compliant, and at midnight Dec. 31, 1999, these PCs will roll back to Jan. 1, 1900.

The Russian agency responsible for these facilities — The Ministry of Atomic Energy (Minatom) — is taking the Y2K problem seriously and, like Los Alamos and the DOE, has developed a plan for its facilities to make sure they're Y2K compliant and that their security systems are up and running into the new year.

In addition to Martinez, members of the DOE team include Rich Roth, Counter Technology Inc., Bethesda, Md., security systems; Chris Abdalla, Aquila Technologies Inc., Albuquerque, computer and network systems; and Jim Coffing, Aquila Technologies Inc., material control and accountability equipment.

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SCIENTISTS PERFECT *IN VITRO* ANALYSIS FOR PLUTONIUM DETECTION

TECHNOLOGY DETECTS EXPOSURE AT LOWER LEVELS FOR RADIOLOGICAL WORKERS

Los Alamos has set a new standard for the monitoring of radiological workers who have a potential for exposure to plutonium. Based on technology used in the nuclear weapons program, scientists have perfected an *in vitro* analysis technique using thermal ionization mass spectrometry, or TIMS. *In vitro* refers to the analysis of materials excreted from the body, in this case urine.

TIMS enables Laboratory analysts in the bioassay program to monitor for a lifetime dose from plutonium down to 0.1 rem — making this technique 40 times more sensitive than the measurement levels associated with existing alpha spectroscopy methods that only can measure a minimum detectable dose of 4 to 6 rem.

TIMS takes bioassay testing to a whole new level, according to Sandy Wagner, bioassay analytical project leader in Los Alamos' Radiochemistry Group. "We implemented the procedure a couple of years ago, and we're now to the point that it's standardized. We've moved into production mode," Wagner said.

Fred Roensch prepares a sample for thermal ionization mass spectrometry. TIMS can measure a plutonium dose with 40 times the sensitivity than alpha spectroscopy methods.

With its ability to measure at the 0.1 rem level, TIMS is the only technology currently available that complies with the latest Department of Energy regulations for *in vitro* bioassay monitoring of plutonium-239.

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Since the days of the Manhattan project, plutonium-worker monitoring was accomplished through alpha spectroscopy — a process that counts the number of alpha particles emitted from a sample.

Alpha spectroscopy, besides being less sensitive, cannot distinguish between the isotopes of plutonium-239 and -240. The ability to make this distinction is important when determining the source of an exposure. For instance, the relative amount of plutonium-239 is different in atmospheric fallout than in weapons components.

TIMS analysis, on the other hand, distinguishes between plutonium-239 and plutonium-240, determining what plutonium isotopes are associated with an exposure and from what source the contamination originated.

Originally used in the nuclear testing program to examine fission yields and products of underground nuclear tests, TIMS works by placing a processed sample onto a filament that is then introduced into the vacuum chamber of a mass spectrometer. The filament is resistively heated, atomizing and ionizing the plutonium sample in the process.

The ions are accelerated through a magnetic field, facilitating separation according to mass, with heavier ions having more momentum. Magnetic field scanning provides momentum focusing of each mass onto an exit slit. Ions of each mass are then detected using a pulse counting detector system.

"We would love to expand our customer base and provide radiological workers throughout the complex with this level of monitoring," Wagner said. At present, the TIMS process is more expensive than alpha spectroscopy because it requires ultrapure materials and a special class of clean room. Costs are expected to come down, though, as the number of samples increases and instruments are automated.

The Laboratory's main customers for bioassay TIMS analysis are internal, but Los Alamos also provides TIMS analysis of soil, water and other materials for the International Atomic Energy Agency, the Nevada Test Site, the Savannah River Ecology Laboratory and others.

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NEW CENTER LOOKS AT WATER RESOURCES IN THE SOUTHWEST

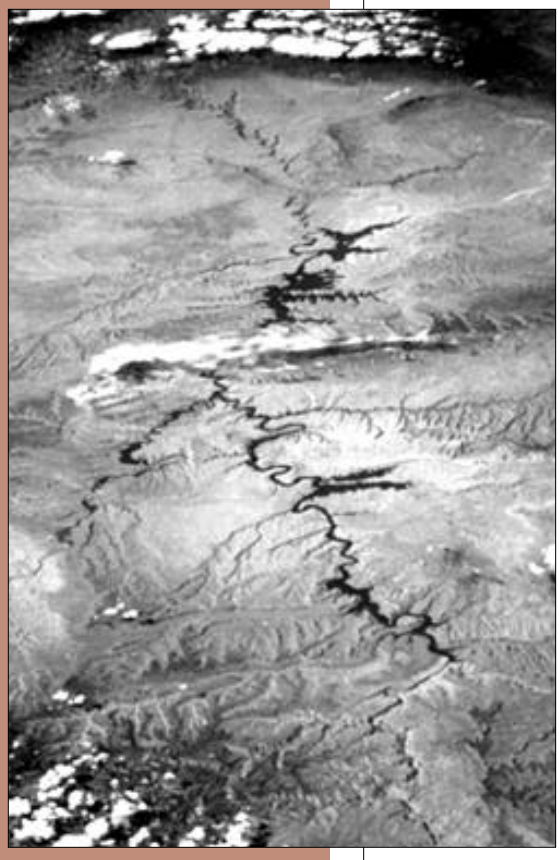
LOS ALAMOS' HIGH-PERFORMANCE COMPUTING CAPABILITIES WILL BE USED IN NATIONAL SCIENCE FOUNDATION PROJECT

As global population growth and economic development place intense demands on water resources, water-management issues in arid regions such as the Southwestern United States grow in importance.

Recognizing this need, the National Science Foundation recently established a Science and Technology Center on the Sustainability of Water Resources in Semi-Arid Regions. The $16 million, five-year project, which is led by the University of Arizona, draws on the expertise of Los Alamos scientists.

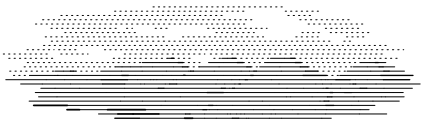
Los Alamos' role will be to develop a computing environment that supports experiments and detailed simulations of the hydrology of large river basins like the Rio Grande or Colorado.

The work will link models to different components of a basin's water cycle. Components will include models of weather, land surface, groundwater hydrology and river networks, as well as such socio-economic elements as agriculture and land use.



This southwestern-looking view taken from the Space Shuttle orbiter Columbia, shows parts of Arizona and Utah. The Colorado and San Juan rivers and Lake Powell are clearly visible.

Photo courtesy of NASA



Los Alamos also will manage the large databases required by detailed basin simulations and support the visualization and analysis of the physics of the hydrological cycle.

The project will give Los Alamos the opportunity to demonstrate its unclassified high-performance computing skills by applying parallel computing and advanced computational techniques to help other researchers improve the efficiency of models.

An important goal of this particular Science and Technology Center is to make the public more “hydrologically literate” and expand people's understanding of the water supply and bring these crucial use issues to the forefront.

The center will bring water-resource management and conservation issues to the forefront of science education at all levels. Activities include K-12 teacher education programs with field study, as well as the development of new curricular materials and special outreach to Native American schools.

The NSF established the Science and Technology Center program in 1987 to respond to a White House commitment to fund research that creates educational opportunities. The program also encourages technology transfer and provides innovative approaches to interdisciplinary research challenges.

Other participants in the Water Resources Science and Technology Center are the New Mexico Institute of Mining and Technology, Pennsylvania State University, the University of California (Los Angeles, Scripps Institution of Oceanography and Riverside), Columbia University, Biosphere 2, the University of New Mexico, Northern Arizona University, the Desert Research Institute, the Instituto Mexicano de Tecnologia del Agua, the Instituto el Medro Ambiente y Desanollo Sustenable del Estado de Sonora, the U.S. Geological Survey, the Agricultural Research Service, the Army Corps of Engineers and the International Boundary and Water Commission.

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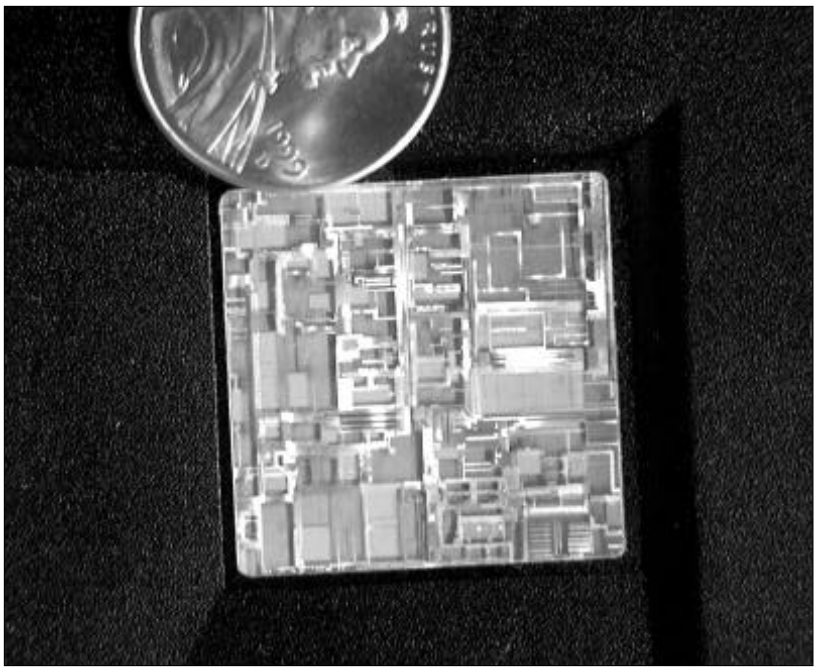
NEW CHIP ON THE BLOCK

LOS ALAMOS TESTS EFFICIENCY OF NEW INTEL PENTIUM III XEON CHIP

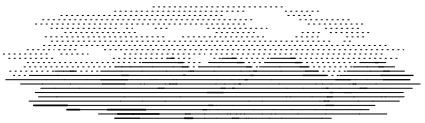
Los Alamos and Intel Corp. are partnering on a project in which the Laboratory tested the efficiency of a new 500 megahertz Intel-developed computer chip.

The agreement to test the chip grew out of a visit several Los Alamos employees made to an Intel Corp. plant in Sacramento, Calif., early this year. The Laboratory was interested in learning if the new Intel chip would improve performance of a shared software system it uses. Intel Corp., in turn, got a first-hand look at how its new computer chip performed under real-world conditions.

The new Pentium III xeon chips were installed in Citrix servers that house the Enterprise Information Applications software used around the Lab. Citrix is used by the Business Information Systems Group to allow Lab employees to access the EIA software from their desktop computers. Business Information Systems ran a complex Microsoft Excel spreadsheet problem to test the chip.



The Laboratory has been testing Pentium III xeon chips for Intel Corp. The chips are similar in size to the Pentium II chip shown here.



While in Sacramento, Intel officials asked if the Laboratory would consider testing the Pentium III xeon chip. The 500 megahertz chip is faster than the current Pentium Pro computer chip in the Compaq NT servers where the Citrix software resides. The faster chip should handle more transactions from Lab employees who use Citrix, according to Los Alamos' Michael Calhoun.

"We can get more concurrent users on a [server] and it is more cost effective for us," Calhoun explained. "And to the individual user, they should see better performance on their end."

In addition to testing the Pentium III xeon chip, Intel wants to send some of its computer network staff to Los Alamos to do a long-term project with the Lab using the UNIX-based LINUX operating system.

"Given our interest and need for ever-increasing processor power and Intel's desire to find sites where the new hardware can really be put to the test, it seems that the fit is good for this initial cooperative venture," said Los Alamos' Bob Newell. "It's a small first step, but should it be successful, it could be the forerunner to additional ventures involving the Laboratory and Intel. Should things continue to move forward, it's bound to be of benefit to both of us."

Los Alamos previously entered into a Cooperative Research and Development Agreement, or CRADA, with Intel. The CRADA dealt with the design of a new process to capture volatile organic compounds, preventing their release into the environment. Volatile organic compounds are a byproduct of the computer chip manufacturing process.

A current CRADA with Intel deals with a modeling and simulation study to improve the performance of computer chips.

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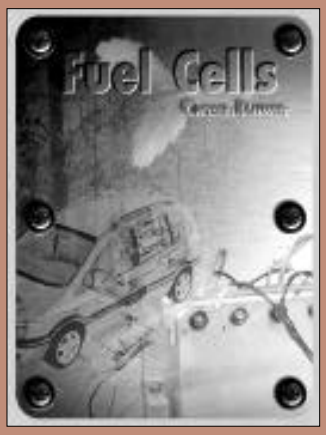
CLEAN AND GREEN

LOS ALAMOS WRITES FUEL CELL TUTORIAL FOR HIGH SCHOOL AND COLLEGE STUDENTS



The Department of Energy is increasingly interested in clean transportation technologies to reduce our dependence on foreign oil, increase energy savings and improve air quality. Research at Los Alamos into fuel cells, a power source that combines hydrogen and oxygen to produce electricity, is helping to commercialize "green" vehicles.

A comprehensive tutorial on fuel cells, written and designed for high school and college students, is now available on the Laboratory's education Web site at http://education.lanl.gov/resources/fuelcells. The 36-page publication and the Web site were featured in the July 30 issue of *Science* magazine, which recommended the guide as an introduction to the subject. Printed copies also are available from the Office of Advanced Automotive Technologies at the Department of Energy.

The tutorial was developed for the DOE office of Advanced Automotive Technologies by Marcia Zalbowitz of the Laboratory's Education Program Office and Sharon Thomas, a recent postdoctoral fellow in the Laboratory's Electronic and Electrochemical Materials and Devices Group.

"The Office of Advanced Automotive Technologies receives many requests from high school and college students who want to learn more about fuel cells, so they asked us to develop materials that could be mailed to students' homes," Zalbowitz said. "What we designed has a narrative text with 'tutorial boxes' that contain more detailed information about specific topics."

The tutorial contains a detailed explanation of what a fuel cell is, focusing on the polymer electrolyte membrane (PEM) technology. These fuel cells operate at relatively low temperatures, have high power density, can vary their output quickly to meet shifts in power demand, and are suitable for transportation applications where quick startup is required.

There also is information about other types of fuel cells and fuels, a brief overview of potential uses for fuel cells and information about areas in need of further research.

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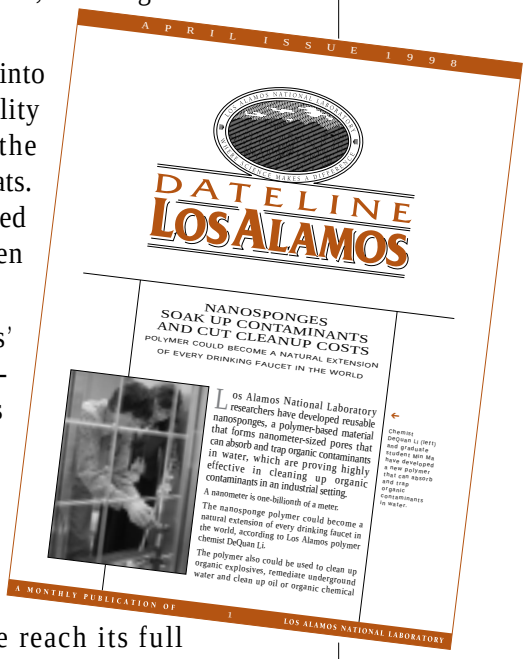
DATELINE FOLLOWUP

LABORATORY LICENSES NANOSPONGE TECHNOLOGY

A new method that could be used to purify home water supplies has been licensed to private industry.

The technology, commonly called a nanosponge, uses a polymer-based material that forms pores about one-billionth of a meter in size that absorb and trap organic contaminants in water, reducing their concentrations to parts-per-trillion levels.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NANOSPONGES SOAK UP CONTAMINANTS AND CUT CLEANUP COSTS

POLYMER COULD BECOME A NATURAL EXTENSION OF EVERY DRINKING FAUCET IN THE WORLD

Los Alamos National Laboratory researchers have developed reusable nanosponges, a polymer-based material that forms nanometer-sized pores that can absorb and trap organic contaminants in water, which are proving highly effective in cleaning up organic contaminants in an industrial setting.

A nanometer is one-billionth of a meter.

The nanosponge polymer could become a natural extension of every drinking faucet in the world, according to Los Alamos polymer chemist DeQuan Li.

The polymer also could be used to clean up organic explosives, remediate underground water and clean up oil or organic chemical

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In addition, nanosponges can be fabricated into granular solids, powders and optical-quality thin films, enabling users to customize the polymer for multiple applications and formats. A simple alcohol rinsing releases the collected contaminants from the polymer, which then can be reused.

DeQuan Li and Min Ma of Los Alamos' Bioscience and Biotechnology Group developed the nanosponge technology, which was featured in the April 1998 issue of *Dateline: Los Alamos*.

"This water filtering technology is very versatile and holds great promise for the home consumer and industrial markets. I look forward to seeing the nanosponge reach its full potential in the coming years," said Li.

The Laboratory's Industrial Business Development Program Office recently signed the exclusive six-month license option agreement with Manhattan Scientifics Inc. to further develop nanoporous polymer water filtering technology for home consumer use. Manhattan Scientifics, whose research headquarters is in Los Alamos, has the option to renew the license for an additional year.

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PEOPLE IN THE NEWS

Neutron scattering pioneer Ferenc Mezei received the first-ever Walter Haelg Prize from the European Neutron Scattering Association. The prize is named for Professor Haelg, the initiator of neutron scattering in Switzerland, who made a generous donation to fund the award. Mezei is the visiting John Wheatley Scholar working in the Los Alamos Neutron Science Center Division. He is developing new spallation techniques to advance areas of neutron scattering normally performed only with nuclear reactors by switching to accelerator-based neutron sources. He also is using neutron scattering techniques to study the dynamic behavior of complex matter. Mezei has made several seminal contributions to neutron scattering of the past three decades, including the introduction of so-called neutron supermirrors and a new kind of spin flipper that can turn the neutron's spin in any direction. He is best known for inventing a high-resolution neutron spectrometry technique called the neutron spin echo method, which has helped researchers to better understand magnetic materials, polymers, proteins, glasses, superconducting vortices, quantum fluids and other condensed matter. Mezei also originated the concept of the long-pulse spallation sources in 1993.

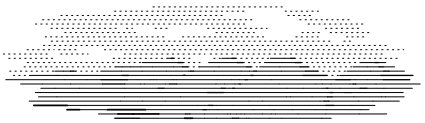
The Department of Defense has awarded Mike Keleher the Defense Meritorious Service Medal for his service with the Defense Threat Reduction Agency. Keleher is a former U.S. Army major who currently works in the Electronic and Electrochemical Materials and Devices Group. He was cited for his management of seven arms control technical development projects while serving as Arms Control Project Officer for the Arms Control Technology Division, On-Site Inspection Directorate, Defense Threat Reduction Agency at Kirtland Air Force Base in Albuquerque. He recently was appointed project leader of the Laboratory's Weapons of Mass Destruction Countermeasures Program, which he will manage on a half-time basis under the DoD Program Office. The new program will focus on providing technology and technical assistance to the government agencies responsible for preventing and responding to threats posed by chemical, biological and high-explosive devices.

DATELINE: LOS ALAMOS

Virginia Rey of Los Alamos' Radiation Protection Services Group has received a Hispanic Heritage Award from the Department of Energy in ceremonies in Washington, D.C. Rey, an 18-year employee of the Laboratory, was honored for her outstanding achievements in providing educational opportunities and other community service activities that impact our nation's youth. The award ceremony coincided with the DOE's kickoff of national Hispanic Heritage Month. Rey has mentored students and other Lab employees, and participated in diversity activities as past chairperson of the Laboratory's Hispanic Diversity Working Group and through the Northern New Mexico chapter of the Society of Mexican-American Engineers and Scientists, of which she currently serves as its vice-president. She was one of several Lab employees recently featured in a special issue of the national magazine that the organization publishes. Rey also is the Environment, Safety and Health Division's student adviser and oversees a program that provides a variety of experiences for ESH students who work at Los Alamos during the summer.

Virginia Rey and Energy Secretary Bill Richardson.
Photo by Charles Watkins, DOE

James Freyer has been selected to serve on the National Institutes of Health's Radiation Study Section. The board is part of the NIH's Center for Scientific Review. Study section members review research grant applications, recommend grant awards to the appropriate NIH national panel and survey the status of research in the field of radiation studies. Members of the Radiation Study Section are selected based on their scientific achievements, as measured by the quality of their research in publications in scientific journals and other research activities and honors. Freyer, who works in the Biosciences Division, will serve on the study section for four years. The 17-year Los Alamos veteran has published 50 peer-reviewed scientific articles and scientific reviews. Freyer has more than 13 years of grant and manuscript review experience, including serving as an ad hoc reviewer for NIH's Radiation, Diagnostic Radiology, Biophysical Chemistry and Pathology B Study Sections. He currently is an ad hoc reviewer for the National Cancer Institute of Canada and routinely reviews manuscripts for more than a dozen scientific journals, including the British Journal of Cancer, Biophysical Journal, Cytometry and Cancer Research. Freyer also is associate editor for The International Journal of Radiation Oncology, Biology and Physics.



DATELINE: LOS ALAMOS

BRIEFLY ...

LOS ALAMOS HAS CREATED A NEW BIOSCIENCE DIVISION, combining all of the Life Sciences Division and parts of the Chemical Science and Technology; Theoretical; and Computing, Information and Communications divisions into a single multidisciplinary organization. Further additions to B Division are anticipated as the organization defines its strategic focus areas and formulates the structure that will provide coordination between line and program opportunities and responsibilities in this field, and strengthen the Lab's position as a national leader in bioscience research. Such efforts include biological agent detection, analysis and identification; deciphering the human genome and understanding how its products function; bioinformatics and computational biology; and the study of biological and chemical systems for technology development. The new division officially came into being in late September. Jill Trewhella, a Laboratory Fellow from CST's Bioscience and Biotechnology Group, and former acting LS Director Scott Cram have been named acting director and deputy director, respectively, for the new division. A national search for a permanent B Division director will start as soon as a Division Director Search Committee is formed.

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